

General introduction to representation theory

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Representation theory

- Method for **simplifying analysis** of a problem in systems possessing some degree of symmetry.
- What is allowed vs. what is not allowed

Keyword : Invariance of the physical properties under application of symmetry operators.



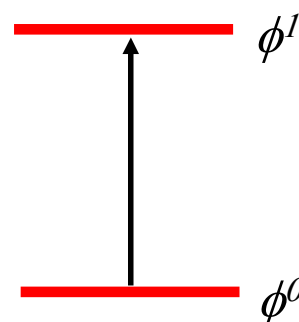
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Spectroscopy

Use to predict vibration spectroscopic transitions that can be observed

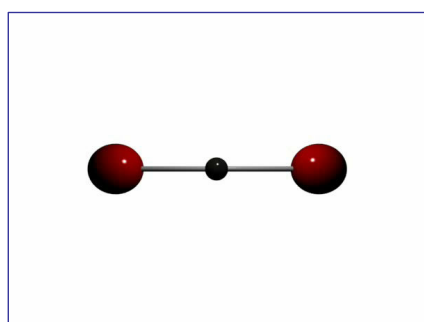
- Ground state characterized by ϕ^0
- Excited state characterized by ϕ^1
- Operator O
- Transition integral :
$$T = \int \phi^0 O \phi^1$$
- The integrand must be invariant under application of all symmetry operations



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IR-Raman active modes

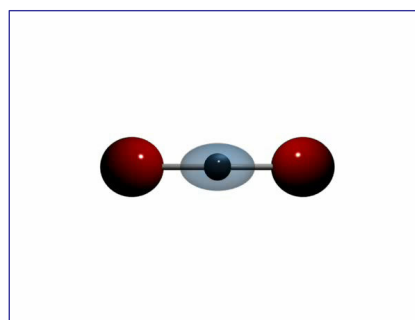
CO₂



IR active, change in dipole moment

$$T = \int \phi^0 \mu \phi^1$$

Dipole moment operator



Raman active, change in polarizability

$$T = \int \phi^0 \alpha \phi^1$$

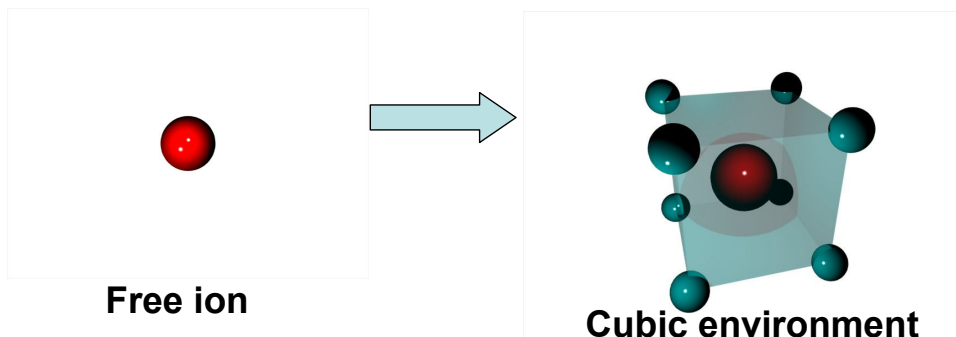
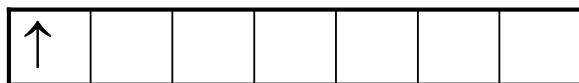
Operator for polarizability



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Crystal field

- Ce^{3+} 4f¹ electronic configuration
- $J=|L-S|=5/2$

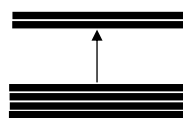


Ground state
multiplet



$$T = \int \phi^0 J_i \phi^1$$

$$\Delta J = 0; +1; -1$$



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MO-LCAO

The molecular orbitals of polyatomic species are linear combinations of atomic orbitals:

$$\Psi = \sum_r c_r \phi_r$$

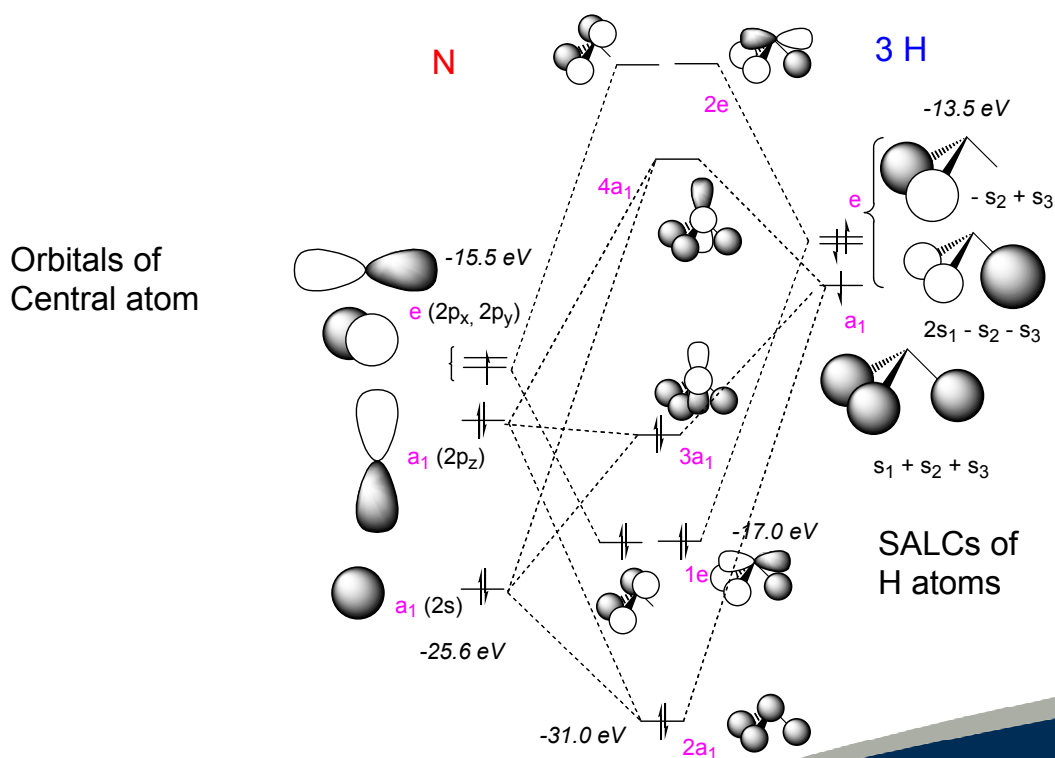
If the molecule has symmetry,
group theory predicts which atomic orbitals can contribute to each molecular orbital.



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MO-LCAO



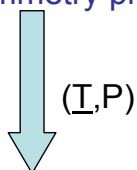
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Phase transitions in solids

Phase transitions often take place between phases of different symmetry.

High symmetry phase, Group G_0

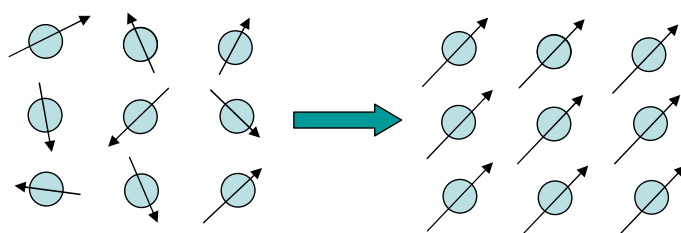


(\mathbb{I}, P)

Low symmetry phase, Group G_1

- This is a “spontaneous” symmetry-breaking process.
- Transition are classified as either 1st order (latent heat) or 2^d order (or continuous)

A simple example: Paramagnetic -> Ferromagnetic transition



“Time-reversal” is lost

- Symmetry under reversal of the electric current



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Landau theory

- Ordering is characterized by a function $\rho(x)$ that changes at the transition.
- Above T_c , $\rho_0(x)$ is invariant under all operations of G_0
- Below T_c , $\rho_1(x)$ is invariant under all operations of G_1

$$\delta\rho = \rho_1 - \rho_0 = \sum_{n'} \sum_i c_i^n \Phi_i^n(x) \longrightarrow \text{Basis functions of irreducible Representation of } G_0.$$

- At $T=T_c$, all the coefficients c_i^n vanish

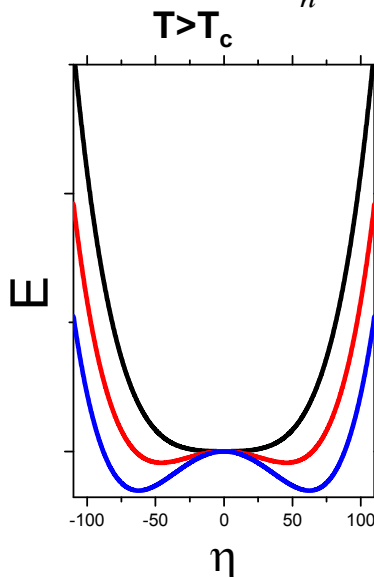


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Landau theory (2)

Φ is invariant under operations of G , each order of the expansion can be written is given by some polynomial invariants of c_i^n .

$$\Phi = \Phi_0 + \sum_{n'} A^n(P, T) \sum_i (c_i^n)^2 + \dots$$



- Thermodynamic equilibrium requires that all A are >0 above T_c .
- In order to have broken symmetry, one A has to change sign at the transition.

$$\Phi = \Phi_0 + \frac{1}{2} a(T)(T - T_c) \eta^2 + C \eta^4 + \dots$$

In a second order phase transition,
a **single symmetry mode** is involved.



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Outline

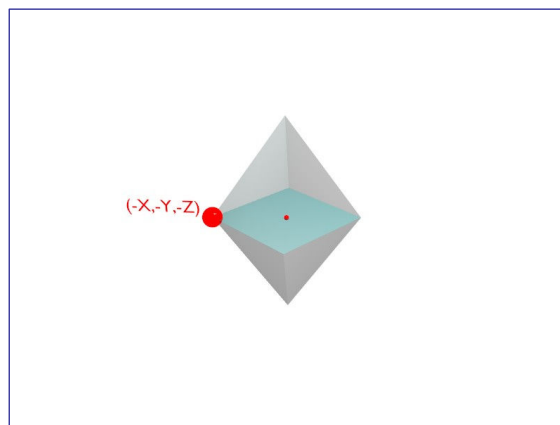
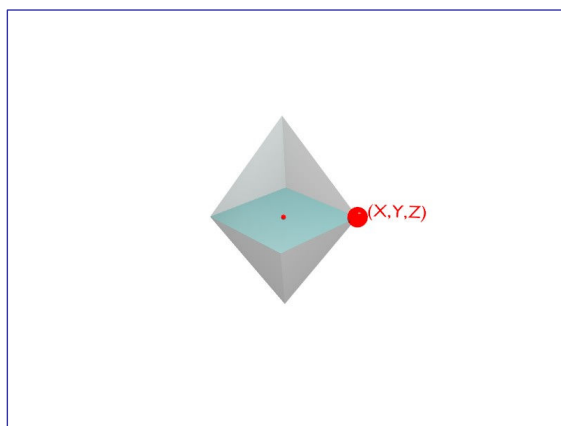
1. Symmetry elements and operations
2. Symmetry groups (molecules)
3. Representation of a group
4. Irreducible representations (IR)
5. Decomposition into IRs
6. Projection
7. Space groups



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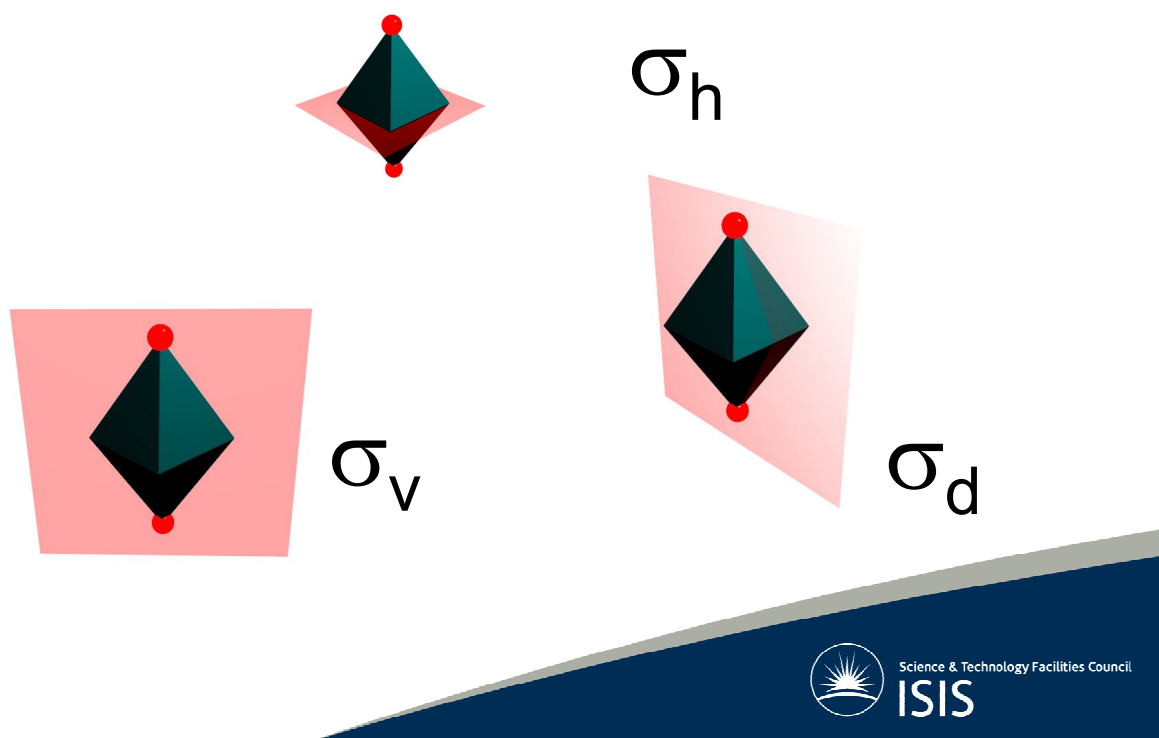
Inversion point $\bar{1}$ ()

Change coordinates of a point (x,y,z) to $(-x,-y,-z)$

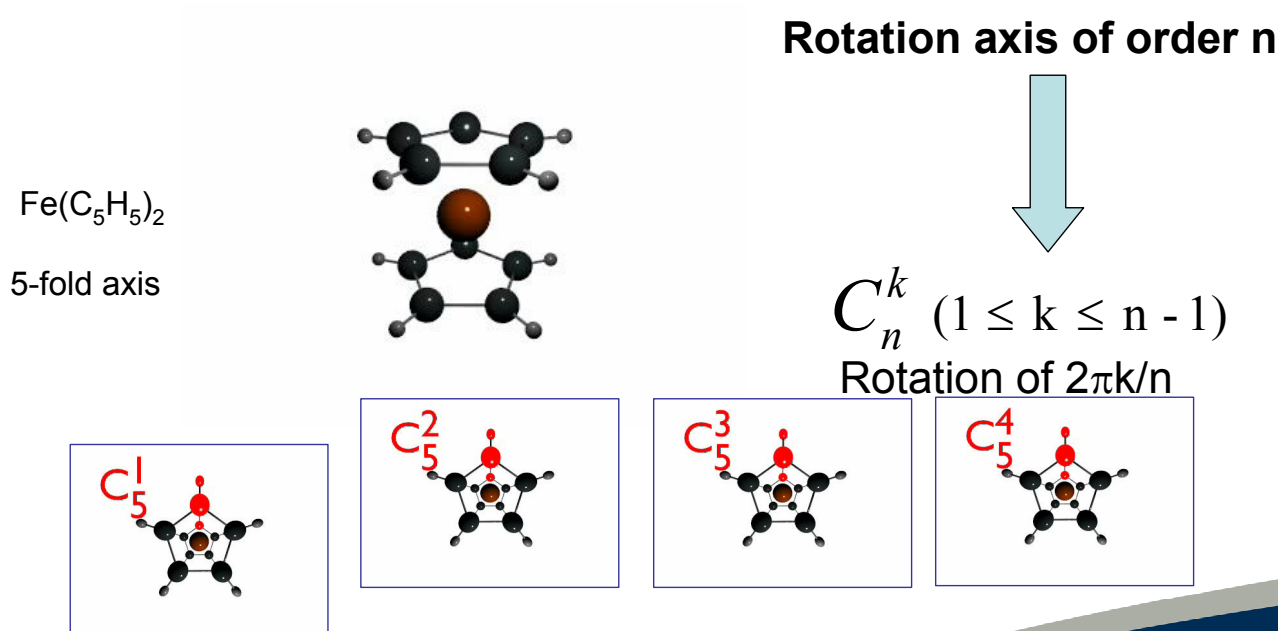


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Mirror planes



Proper rotation C_n (n)

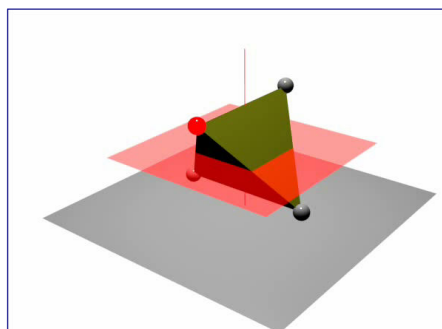
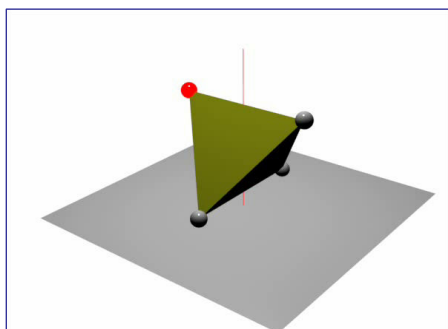


Improper rotation $S_n(\bar{n})$

Combination of two successive operations:

- 1) Rotation C_n around an axis.
- 2) Mirror operation in a plane perpendicular to rotation axis

S_4 in tetrahedral geometry



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Group structure

- Collection of elements for which an associative law of combination is defined and such that for any pair of elements g and h , the product gh is also element of the collection
- It contains a unitary element, E, such that $gE=g$
- Every element g has an inverse, noted g^{-1} such that $gg^{-1}=E$.

The order of a group is simply the number of elements in a group.
We will note the order of a group h .

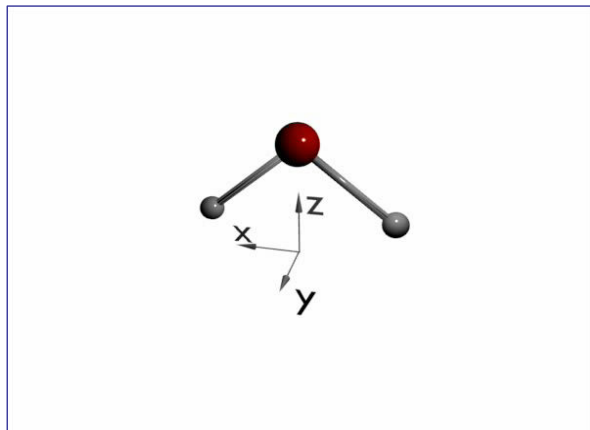


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Multiplication table

Four different operations:

- E
- $\sigma(xz)$
- $\sigma(yz)$
- $C_2(z)$



	E	$C_2(z)$	$\sigma(xz)$	$\sigma(yz)$
E	E	$C_2(z)$	$\sigma(xz)$	$\sigma(yz)$
$C_2(z)$	$C_2(z)$	E	$\sigma(yz)$	$\sigma(xz)$
$\sigma(xz)$	$\sigma(xz)$	$\sigma(yz)$	E	$C_2(z)$
$\sigma(yz)$	$\sigma(yz)$	$\sigma(xz)$	$C_2(z)$	E



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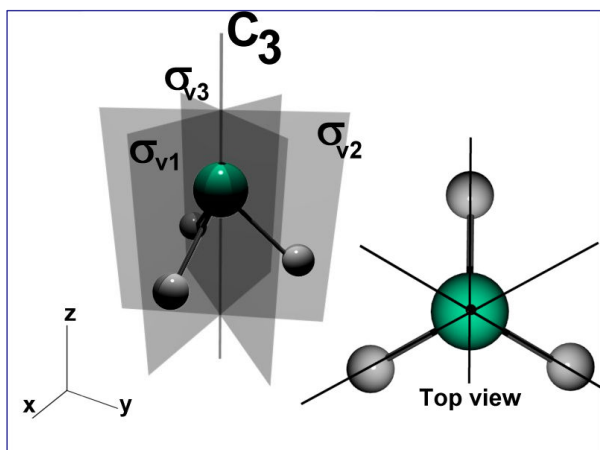
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Classes

Similarity transform: $h = x^{-1}gx$

g and h are conjugate

The set of elements that are all conjugate to one another is called a (conjugacy) class.



Symmetry operations:

$$E, C_3^1, C_3^2, \sigma_{v1}, \sigma_{v2}, \sigma_{v3}$$

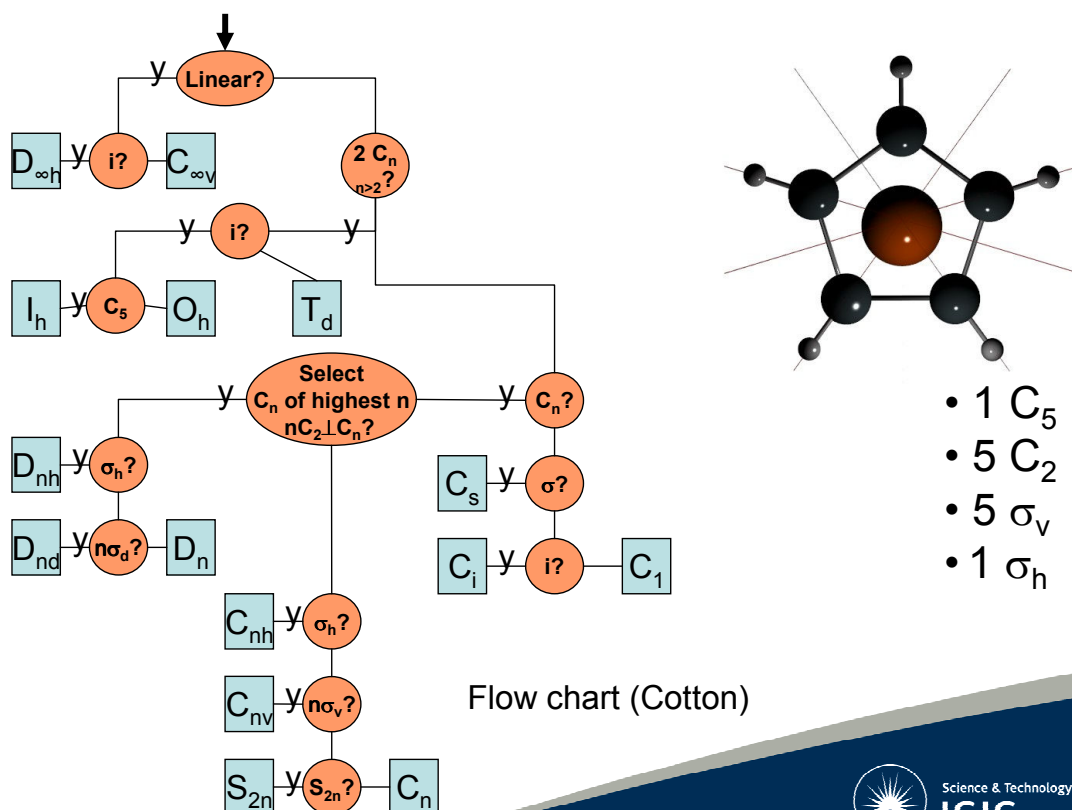
$$\sigma_{v1}^{-1} C_3^1 \sigma_{v1} = C_3^2$$



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Determination of G



Representation of G

A group G is represented in a vector space E , of dimension n , if we form an homomorphism D from G to $GL_n(E)$:

$$\forall g \in G, g \mapsto D(g) \in GL_n(E)$$

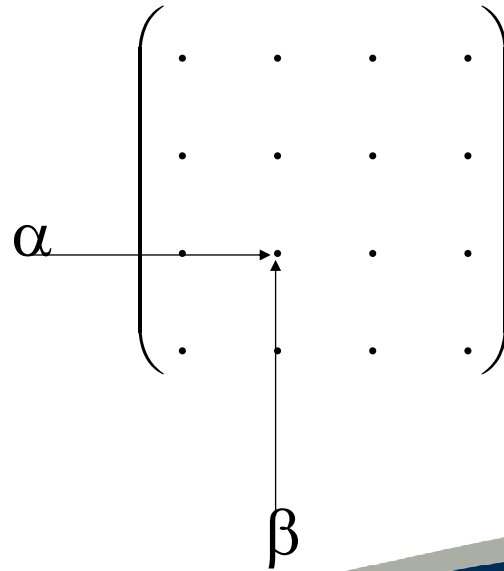
$$\forall g, g' \in G, D(gg') = D(g)D(g')$$

$$D(1) = 1$$

$$\forall g \in G, D(g^{-1}) = (D(g))^{-1}$$

Matrices

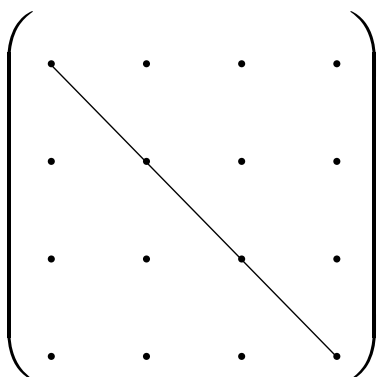
- If a basis of E is chosen, then we can write $D(g)$ as n by n matrices.
- We will note $D_{\alpha\beta}(g)$ the matrix elements (line α , row β)



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Character



The trace (sum of diagonal elements) is noted χ .

$$\chi(g) = \sum_{\alpha} D_{\alpha\alpha}(g)$$

Important reminder :

$$D' = P^{-1}DP$$

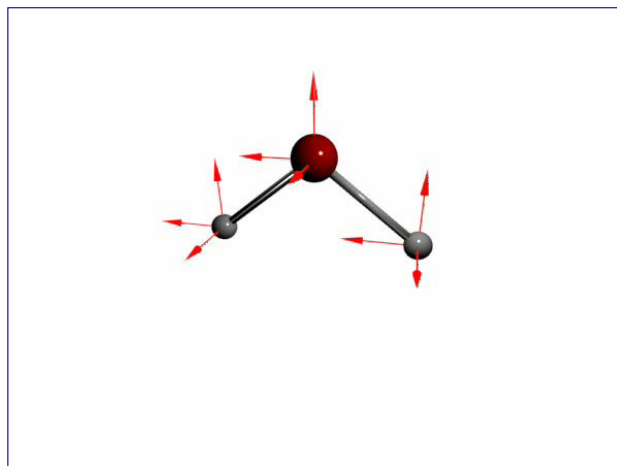
Matrices that are conjugate to one another have the same trace.



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Example : H₂O modes



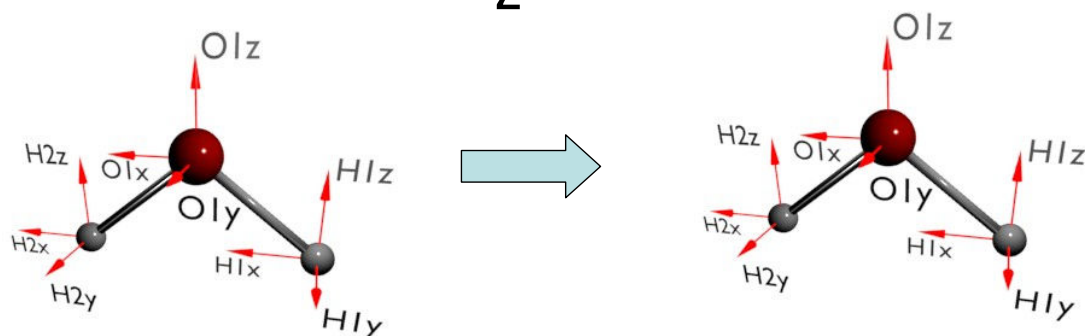
A symmetry operation produces linear transformations in the vector space E.



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H₂O- E



$$\begin{pmatrix} H1x' \\ H1y' \\ H1z' \\ H2x' \\ H2y' \\ H2z' \\ O1x' \\ O1y' \\ O1z' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} H1x \\ H1y \\ H1z \\ H2x \\ H2y \\ H2z \\ O1x \\ O1y \\ O1z \end{pmatrix}$$

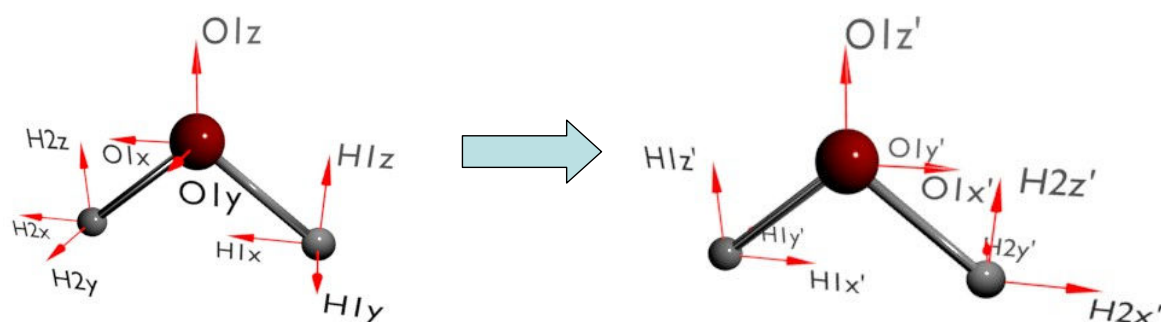
$$\chi(E)=9$$



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H₂O- C₂-axis



$$\begin{pmatrix} H1x' \\ H1y' \\ H1z' \\ H2x' \\ H2y' \\ H2z' \\ O1x' \\ O1y' \\ O1z' \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} H1x \\ H1y \\ H1z \\ H2x \\ H2y \\ H2z \\ O1x \\ O1y \\ O1z \end{pmatrix}$$

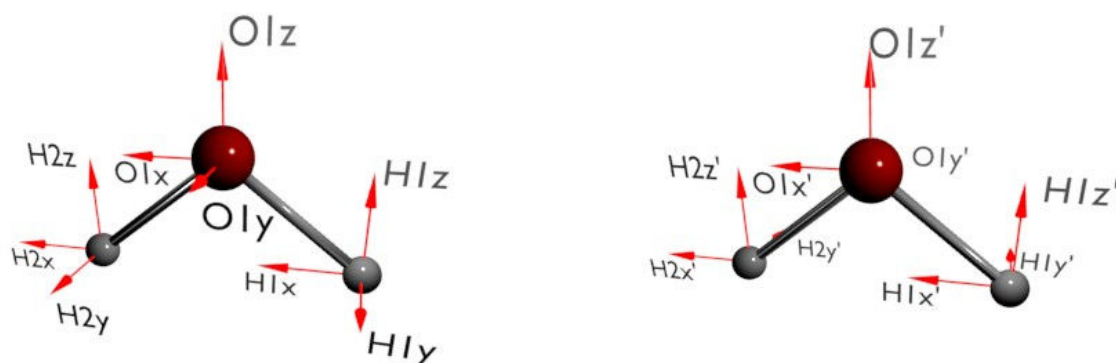
$$\chi(C_2) = -1$$



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H₂O-σ(xz)



$$\begin{pmatrix} H1x' \\ H1y' \\ H1z' \\ H2x' \\ H2y' \\ H2z' \\ O1x' \\ O1y' \\ O1z' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} H1x \\ H1y \\ H1z \\ H2x \\ H2y \\ H2z \\ O1x \\ O1y \\ O1z \end{pmatrix}$$

$$\chi(\sigma(xz)) = 3$$



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Matrix multiplication

$$\sigma(xz) \times C_2(z) = \sigma(yz)$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$



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Irreducible representations (IRs)

D is a representation of a group in a space E.

D is reducible if it leaves **at least one subspace** of E invariant, otherwise the representation is irreducible.

$$E = \sum_{\oplus} E_i = E_1 \oplus E_2 \dots$$

Every element of E can be written in one and only one way as a sum of elements of E_i .



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IRs

- In matrix terms:

A representation is reducible if one can find a similarity transformation (change of basis) that send all the matrices $D(g)$ to the same block-diagonal form.

$$\begin{pmatrix} \boxed{\text{diagonal}} & & 0 \\ & \boxed{\text{diagonal}} & \\ 0 & & \boxed{\text{diagonal}} \end{pmatrix}$$



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Properties of block diagonal matrices

$$\begin{matrix} D_1 & & D_2 \\ \left(\begin{array}{cc} \boxed{\text{yellow}} & 0 \\ 0 & \boxed{\text{green}} \end{array} \right) & \times & \left(\begin{array}{cc} \boxed{\text{yellow}} & 0 \\ 0 & \boxed{\text{green}} \end{array} \right) & = & \left(\begin{array}{cc} \boxed{\text{yellow}} & 0 \\ 0 & \boxed{\text{green}} \end{array} \right) \end{matrix}$$

Corresponding blocks are multiplied separately.



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IRs

- In a finite group, there is a limited number of IRs.

$$\sum_i (l_i)^2 = h$$

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0



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Character tables

- In a finite group, there is a limited number of IRs.
- IRs are described in character tables:

A table that list the symmetry operations horizontally, IRs labels vertically and corresponding characters.

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0



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Great Orthogonality theorem

- For two given IRs D^i and D^j , of dimension l_i and l_j respectively.

$$\sum_{g \in G} D_{\alpha\beta}^i(g) D_{\alpha'\beta'}^j(g)^* = \frac{h}{\sqrt{l_i l_j}} \delta_{ij} \delta_{\alpha\alpha'} \delta_{\beta\beta'}$$

$$\sum_{g \in G} (\chi^i(g))^2 = h$$

$$\sum_{g \in G} \chi^i(g) \chi^j(g) = 0$$



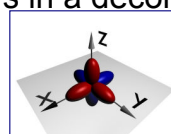
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GOT

D is a reducible representation.

The number of times that a representation i appears in a decomposition is :

$$n_i = \frac{1}{h} \sum_{g \in G} \chi_i(g)^* \chi(g)$$



C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0
D	3	0	1

$$n_{A_1} = 1/6(3*1 + 2*1*0 + 3*1*1) = 1$$

$$n_{A_2} = 1/6(3*1 + 2*1*0 + 3*-1*1) = 0$$

$$n_E = 1/6(3*1 + 2*-1*0 + 3*0*1) = 1$$



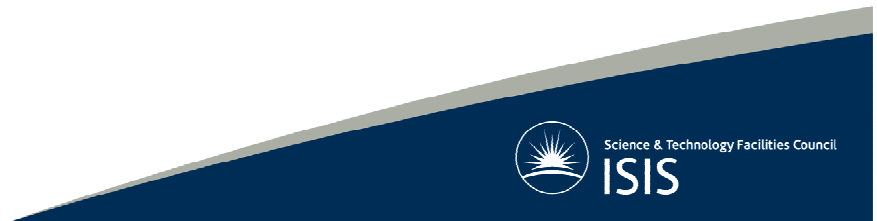
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Projection

- Project a vector of the vector space into the space of the IR to find the symmetry adapted vectors.

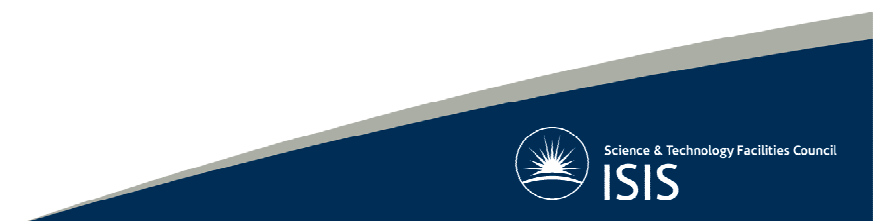
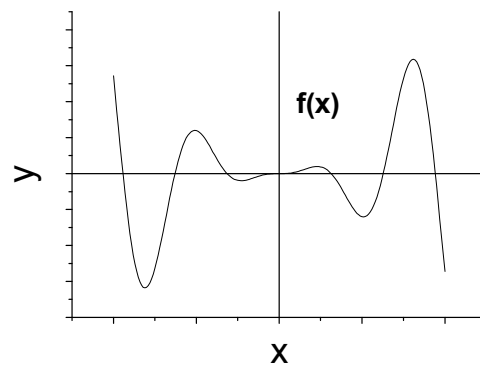
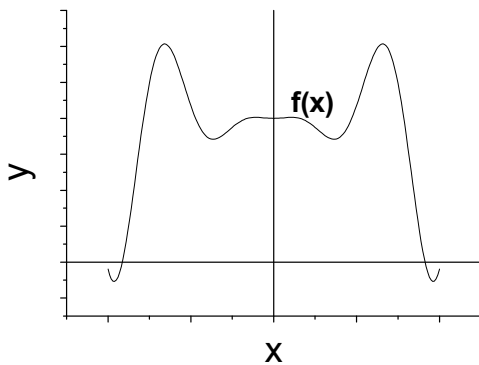
$$\hat{P}_{\lambda}^{\nu} = \sum_{g \in G} D_{\lambda\mu}(g)^* \hat{g}$$

* indicates complex conjugate



Integrals

$$\int_{-\infty}^{\infty} f(x) dx$$



Space group Symmetry operations

- Use the Seitz notation $\{\alpha|\mathbf{t}_\alpha\}$
- α rotational part (proper or improper)
- \mathbf{t}_α translational part

$$\{\alpha|\mathbf{t}_\alpha\} \{\beta|\mathbf{t}_\beta\} = \{\alpha\beta|\alpha\mathbf{t}_\beta + \mathbf{t}_\alpha\}$$

Space group: infinite number of symmetry operations

Diagrammatic symbol or complete name	Graphical symbol	Matrix symbol of a right-handed coordinate system of the three-dimensional vectors parallel to the axes	Point symbol (space group)
Identity		None	1
Two-fold rotation axis		None	2
Three-fold rotation axis		None	3
Four-fold rotation axis		None	4
Six-fold rotation axis		None	6
Two-fold rotation axis with center of symmetry		None	2/m
Three-fold rotation axis with center of symmetry		None	3/m
Four-fold rotation axis with center of symmetry		None	4/m
Six-fold rotation axis with center of symmetry		None	6/m
Two-fold rotation axis with center of symmetry and glide plane		None	2/m, 2/m, 2/m
Three-fold rotation axis with center of symmetry and glide plane		None	3/m, 3/m, 3/m
Four-fold rotation axis with center of symmetry and glide plane		None	4/m, 4/m, 4/m
Six-fold rotation axis with center of symmetry and glide plane		None	6/m, 6/m, 6/m
Two-fold rotation axis with center of symmetry and glide plane and screw axis		None	2/m, 2/m, 2/m, 2/m
Three-fold rotation axis with center of symmetry and glide plane and screw axis		None	3/m, 3/m, 3/m, 3/m
Four-fold rotation axis with center of symmetry and glide plane and screw axis		None	4/m, 4/m, 4/m, 4/m
Six-fold rotation axis with center of symmetry and glide plane and screw axis		None	6/m, 6/m, 6/m, 6/m

Symmetry plane or symmetry line	Graphical symbol	Glide vector is such of lattice translation vectors parallel and normal to the projection plane	Point symbol
Symmetry plane or symmetry line		None	m
Reflection plane, mirror plane		None	m
Reflection line, mirror line (two dimensions)		None	m
'Axial' glide plane		Lattice vector along line in projection plane	a, b or c
Glide line (two dimensions)		Lattice vector along line in figure plane	a, b or c
'Axial' glide plane		Lattice vector normal to projection plane	a, b or c
'Diagonal' glide plane (in centred cells only)		Two glide vectors	c
'Diagonal' glide plane		One glide vector with two components	a
'Diamond' glide plane (space of planes, in centred cells only)		One glide vector with two components, one along line parallel to projection plane, one normal to projection plane	d



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Group of translation T

T	$\{1 000\} \{1 100\} \{1 010\} \{1 t\} \{1 200\} \dots\dots\dots$
Γ^K	$\dots\dots\dots e^{-ikt}$

- Infinite **abelian** group
- Infinite number of irreducible representations, and consists of the complex root of unity.

Basis are Bloch functions.

$$\Phi^k(r) = u_k(r).e^{ikr}$$

$$u_k(r+t) = u_k(r) \quad (t \text{ is a lattice translation})$$

$$\{1|t\}\Phi^k(r) = \Phi^k(r-t) = u_k(r-t).e^{ik(r-t)} = e^{-ikt}\Phi^k(r)$$



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Space group

Consider a symmetry element $g=\{h|t\}$ and a Bloch-function Φ' :

$$\phi^k(r) = u_k(r)e^{ikr}$$

$$\phi' = \{h|t\}\phi^k(r)$$

$$\{1|u\}\phi' = \{1|u\}\{h|t\}\phi^k(r)$$

$$= \{h|t\}\{1|h^{-1}u\}\phi^k(r)$$

$$= \{h|t\}e^{-ikh^{-1}u}\phi^k(r) = e^{-ikh^{-1}u}\{h|t\}\phi^k(r) = e^{-i(hk)u}\phi'$$

Φ' is a bloch function $\Phi^{hk}(r)$



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Little group G_k

- By applying the rotational part of the symmetry elements of the paramagnetic group, one finds a set of k vectors, known as the “star of k ”
- Two vectors k_1 and k_2 are *equivalent* if they equal or related by a reciprocal lattice vector.
- In the general case, if all vectors k_1, k_2, \dots, k_i in the star are not equivalent, the functions Φ_{k_i} are linearly independent.
- The group generated from the point group operations that leave k invariant elements + translations is called the group of the propagation vector k or little group and noted G_k .
- In G_k , the functions Φ_{k_i} are not all linearly independent, and the representation is reducible.



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IRs of G_k

$$g \in G_k$$

$$D(g) = D_{pr}(h) e^{i \cdot 2 \cdot \pi \cdot \mathbf{k} \cdot \mathbf{t}}$$

Tabulated (Kovalev tables) or calculable for all space group and all \mathbf{k} vectors **for finite sets of point group elements h**



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Despite the **infinite number** of atomic positions in a crystal symmetry elements in a space group

...a representation theory of space groups is feasible using **Bloch functions** associated to \mathbf{k} points of the reciprocal space. This means that the group properties can be given by matrices of finite dimensions for the

- **Reducible (physical) representations** can be constructed on the space of the components of a set of generated points in the zero cell.
- **Irreducible representations** of the Group of vector \mathbf{k} are constructed from a finite set of elements of the zero-block.

Orthogonalization procedures explained previously can be employed to construct symmetry adapted functions



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Symmetry analysis

Example 1



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- Space group $P4mm$, $k=0$, Magnetic site $2c$

International Tables for Crystallography (2006). Vol. A, Space group 99, pp. 382–383.

$P4mm$

C_{4v}^1

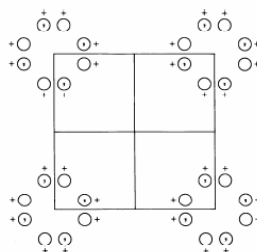
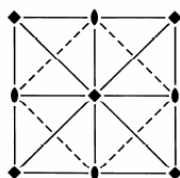
$4mm$

Tetragonal

No. 99

$P4mm$

Patterson symmetry $P4/mmm$



Origin on $4mm$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$; $x \leq y$

Symmetry operations

- | | | | |
|-----------------|-----------------|-----------------------|-----------------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) 4^+ $0,0,z$ | (4) 4^- $0,0,z$ |
| (5) m $x,0,z$ | (6) m $0,y,z$ | (7) m x,\bar{x},z | (8) m x,x,\bar{z} |



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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

General:

no conditions

Special:

no extra conditions

no extra conditions

no extra conditions

$hkl : h+k=2n$

no extra conditions

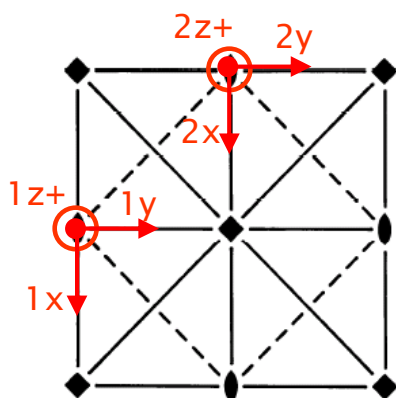
no extra conditions

8	<i>g</i>	1	(1) x,y,z (5) x,\bar{y},z	(2) \bar{x},\bar{y},z (6) \bar{x},y,z	(3) \bar{y},x,z (7) \bar{y},\bar{x},z	(4) y,\bar{x},z (8) y,x,z
4	<i>f</i>	. <i>m</i> .	$x, \frac{1}{2}, z$	$\bar{x}, \frac{1}{2}, z$	$\frac{1}{2}, x, z$	$\frac{1}{2}, \bar{x}, z$
4	<i>e</i>	. <i>m</i> .	$x, 0, z$	$\bar{x}, 0, z$	$0, x, z$	$0, \bar{x}, z$
4	<i>d</i>	. . <i>m</i>	x, x, z	\bar{x}, \bar{x}, z	\bar{x}, x, z	x, \bar{x}, z
2	<i>c</i>	2 <i>m m</i> .	$\frac{1}{2}, 0, z$	$0, \frac{1}{2}, z$		
1	<i>b</i>	4 <i>m m</i>	$\frac{1}{2}, \frac{1}{2}, z$			
1	<i>a</i>	4 <i>m m</i>	$0, 0, z$			



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$\{1|000\}$

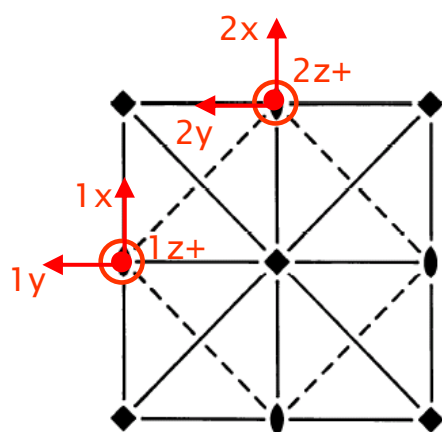


$$\begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{pmatrix}$$



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$\{2_z|000\}$



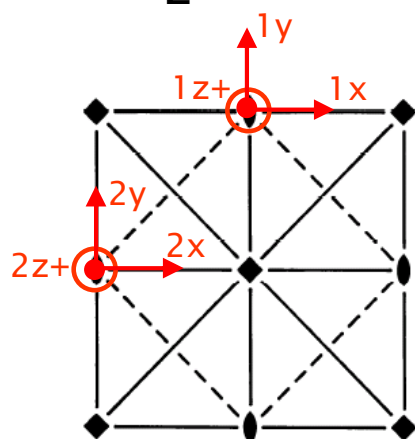
$$\begin{pmatrix} -1 & & & & & \\ & -1 & & & & \\ & & 1 & & & \\ & & & -1 & & \\ & & & & -1 & \\ & & & & & 1 \end{pmatrix}$$



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$\{4_z^+|000\}$



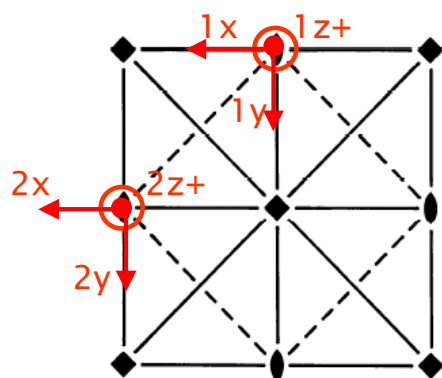
$$\begin{pmatrix} & & -1 & \\ & 1 & & \\ & & & 1 \\ -1 & & & \\ 1 & & 1 & \end{pmatrix}$$



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$$\{4_z|000\}$$



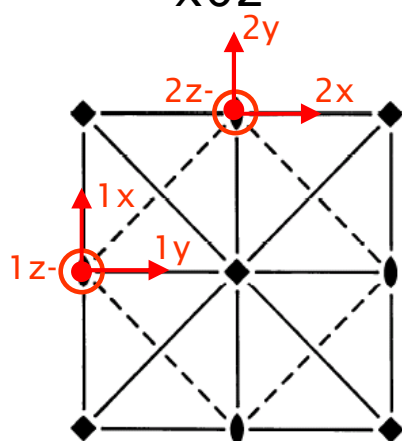
$$\begin{pmatrix} & & 1 \\ & -1 & \\ & & 1 \\ -1 & & \end{pmatrix}$$



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$$\{m_{x0z}|000\}$$



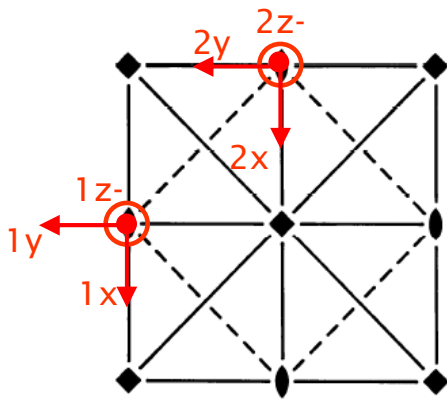
$$\begin{pmatrix} -1 & & & & \\ & 1 & & & \\ & & -1 & & \\ & & & -1 & \\ & & & & 1 \\ & & & & & -1 \end{pmatrix}$$



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$$\{m_{0yz}|000\}$$



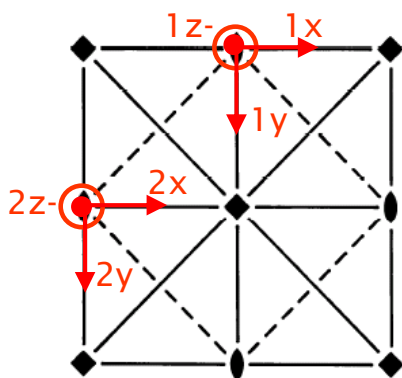
$$\begin{pmatrix} 1 & & & & & \\ & -1 & & & & \\ & & -1 & & & \\ & & & 1 & & \\ & & & & -1 & \\ & & & & & -1 \end{pmatrix}$$



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$$\{m_{x-xz}|000\}$$

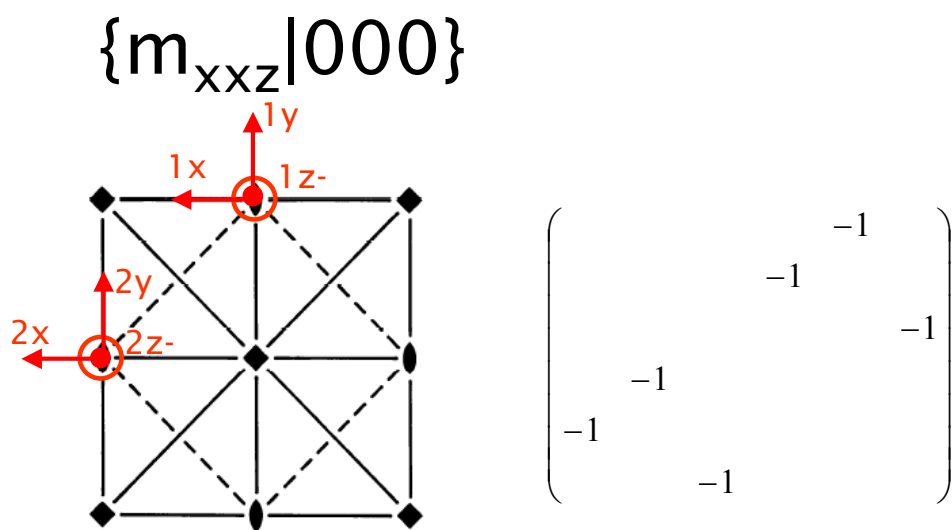


$$\begin{pmatrix} & & & 1 & & \\ & & 1 & & & \\ & & & & & -1 \\ 1 & & & & & \\ & 1 & & & & \\ & & -1 & & & \end{pmatrix}$$



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IRs

IRs/SO	$\{1 000\}$	$\{2_{00z} 000\}$	$\{4_{+00z} 000\}$	$\{4_{-00z} 000\}$	$\{m_{x0z} 000\}$	$\{m_{0yz} 000\}$	$\{m_{x-xz} 000\}$	$\{m_{xxz} 000\}$
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	-1	-1	-1	-1
Γ_3	1	1	-1	-1	1	1	-1	-1
Γ_4	1	1	-1	-1	-1	-1	1	1
Γ_5	1 0 0 1	-1 0 0 -1	i 0 0 -i	-i 0 0 i	0 1 1 0	0 -1 -1 0	0 -i i 0	0 i -i 0
$\chi(\Gamma)$	6	-2	0	0	-2	-2	0	0



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Decomposition into IRs

$$\eta(\Gamma_1) = \frac{1}{8}(6 \times 1 - 2 \times 1 + 0 \times 1 + 0 \times 1 - 2 \times 1 - 2 \times 1 + 0 \times 1 + 0 \times 1) = 0$$

$$\eta(\Gamma_2) = \frac{1}{8}(6 \times 1 - 2 \times 1 + 0 \times 1 + 0 \times 1 - 2 \times -1 - 2 \times -1 + 0 \times -1 + 0 \times -1) = 1$$

$$\eta(\Gamma_3) = \frac{1}{8}(6 \times 1 - 2 \times 1 + 0 \times -1 + 0 \times -1 - 2 \times 1 - 2 \times 1 + 0 \times -1 + 0 \times -1) = 0$$

$$\eta(\Gamma_4) = \frac{1}{8}(6 \times 1 - 2 \times 1 + 0 \times -1 + 0 \times -1 - 2 \times -1 - 2 \times -1 + 0 \times 1 + 0 \times 1) = 1$$

$$\eta(\Gamma_5) = \frac{1}{8}(6 \times 2 - 2 \times -2 + 0 \times 0 + 0 \times 0 - 2 \times 0 - 2 \times 0 + 0 \times 0 + 0 \times 0) = 2$$

$$\Gamma = \Gamma_2 \oplus \Gamma_4 \oplus 2\Gamma_5$$



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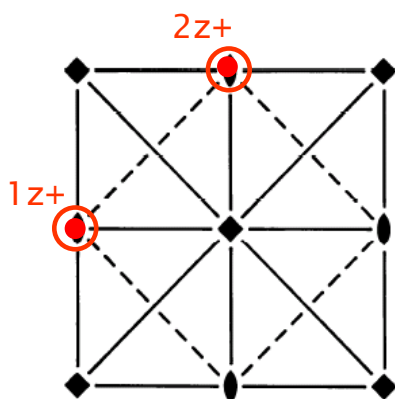
ISIS

Projection onto Γ_2

$$P|1x\rangle = |1x\rangle - |1x\rangle + |2y\rangle - |2y\rangle + |1x\rangle - |1x\rangle - |2y\rangle + |2y\rangle = 0$$

$$P|1y\rangle = |1y\rangle - |1y\rangle - |2x\rangle + |2x\rangle - |1y\rangle + |1y\rangle - |2x\rangle + |2x\rangle = 0$$

$$P|1z\rangle = |1z\rangle + |1z\rangle + |2z\rangle + |2z\rangle + |1z\rangle + |1z\rangle + |2z\rangle + |2z\rangle = 4(|1z\rangle + |2z\rangle)$$



Shubnikov notation $P4m'm'$



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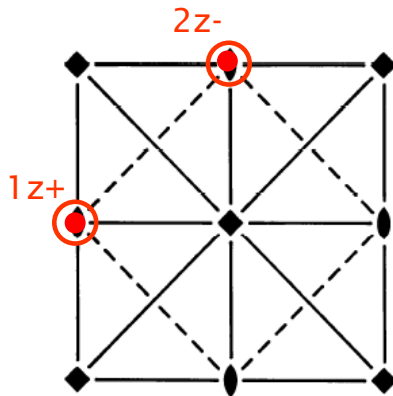
ISIS

Projection onto Γ_4

$$P|1x\rangle = |1x\rangle - |1x\rangle - |2y\rangle + |2y\rangle + |1x\rangle - |1x\rangle + |2y\rangle - |2y\rangle = 0$$

$$P|1y\rangle = |1y\rangle - |1y\rangle + 2|x\rangle - 2|x\rangle - |1y\rangle + |1y\rangle + |2x\rangle - |2x\rangle = 0$$

$$P|1z\rangle = |1z\rangle + |1z\rangle - |2z\rangle - |2z\rangle + |1z\rangle + |1z\rangle - |2z\rangle - |2z\rangle = 4(|1z\rangle - |2z\rangle)$$



Shubnikov notation $P4'mm'$



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Projection onto Γ_5

Projection using the (1,1) elements of the matrices

$$P|1x\rangle = |1x\rangle + |1x\rangle - i|2y\rangle - i|2y\rangle = 2(|1x\rangle - i|2y\rangle)(\phi_1)$$

$$P|1y\rangle = |1y\rangle + |1y\rangle + i|2x\rangle + i|2x\rangle = 2(|1y\rangle + i|2x\rangle)(\phi_2)$$

$$P|1z\rangle = |1z\rangle - |1z\rangle - i|2z\rangle + i|2z\rangle = 0$$

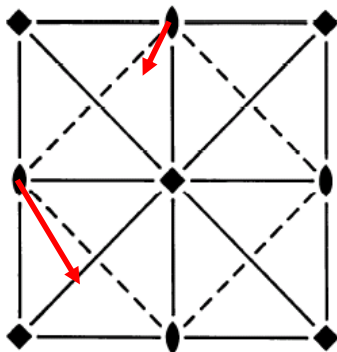
$$P|2x\rangle = |2x\rangle + |2x\rangle - i|1y\rangle - i|1y\rangle = 2(|2x\rangle - i|1y\rangle)(i\phi_2)$$

$$P|2y\rangle = |2y\rangle + |2y\rangle + i|1x\rangle + i|1x\rangle = 2(|2y\rangle + i|1x\rangle)(-i\phi_1)$$

Projection using the (2,2) elements of the matrices

$$P|1x\rangle = 2(|1x\rangle + i|2y\rangle)(\phi_3)$$

$$P|1y\rangle = 2(|1y\rangle - i|2x\rangle)(\phi_4)$$



The magnetic modes can be any linear combinations of $\phi_1, \phi_2, \phi_3, \phi_4$



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Symmetry analysis

Example 2



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• Space group $P2_1/m$, $k=(0,\delta,0)$ Magnetic site 4f

$P2_1/m$

C_{2h}^2

$2/m$

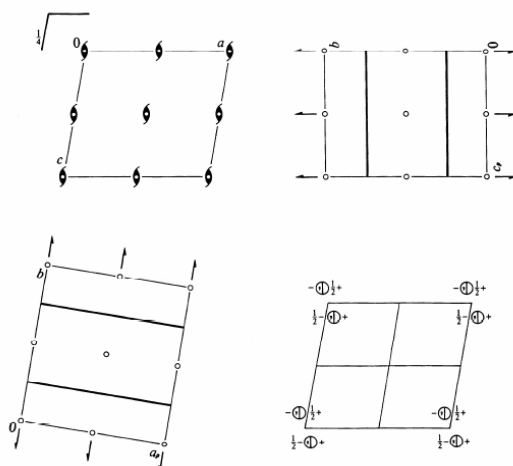
Monoclinic

No. 11

$P12_1/m1$

Patterson symmetry $P12_1/m1$

UNIQUE AXIS b



Origin at $\bar{1}$ on 2_1

Asymmetric unit $0 \leq x \leq 1; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

(1) 1 (2) $2(0, \frac{1}{2}, 0)$ (3) $\bar{1}$ (4) m $x, \frac{1}{2}, z$



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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

General:

$0k0 : k = 2n$

Special: as above, plus

no extra conditions

$hkl : k = 2n$

$hkl : k = 2n$

$hkl : k = 2n$

$hkl : k = 2n$

4	<i>f</i>	1	(1) x, y, z	(2) $\bar{x}, y + \frac{1}{2}, \bar{z}$	(3) $\bar{x}, \bar{y}, \bar{z}$	(4) $x, \bar{y} + \frac{1}{2}, z$
---	----------	---	---------------	---	---------------------------------	-----------------------------------

2	<i>e</i>	<i>m</i>	$x, \frac{1}{4}, z$	$\bar{x}, \frac{3}{4}, \bar{z}$
---	----------	----------	---------------------	---------------------------------

2	<i>d</i>	$\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
---	----------	-----------	-------------------------------	---

2	<i>c</i>	$\bar{1}$	$0, 0, \frac{1}{2}$	$0, \frac{1}{2}, \frac{1}{2}$
---	----------	-----------	---------------------	-------------------------------

2	<i>b</i>	$\bar{1}$	$\frac{1}{2}, 0, 0$	$\frac{1}{2}, \frac{1}{2}, 0$
---	----------	-----------	---------------------	-------------------------------

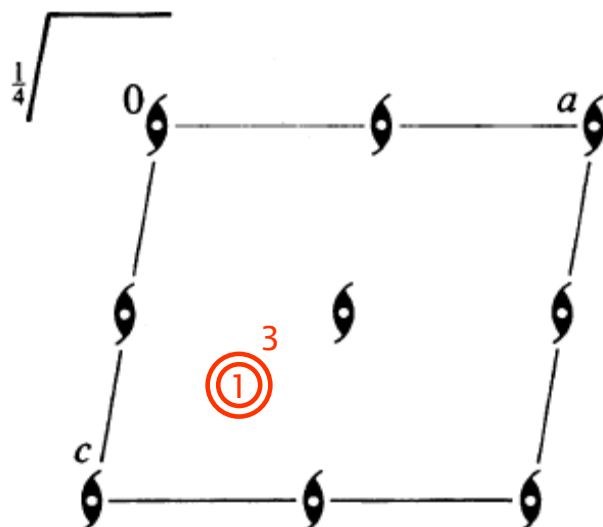
2	<i>a</i>	$\bar{1}$	$0, 0, 0$	$0, \frac{1}{2}, 0$
---	----------	-----------	-----------	---------------------



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②⁴



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Little Group G_K

Operation of the point group on the propagation vector

- Identity $\rightarrow k=(0,\delta,0)$
- 2-fold axis $\rightarrow k=(0,\delta,0)$
- Inversion $\rightarrow -k=(0,-\delta,0)$
- Mirror $\rightarrow -k=(0,-\delta,0)$
- Only $\{1|000\}$ and $\{2_y|0\frac{1}{2}0\}$ belong to G_K
- 4f sites are split into two orbits : (1,2) and (3,4) since no operations of G_K transform sites of the first orbit into that of the second orbit



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IRs of G_K

IRs/SO	$\{1 000\}$	$\{2_y 0\frac{1}{2}0\}$
--------	-------------	-------------------------

Γ_1	1	$e^{i\pi\delta}$
------------	---	------------------

Γ_2	1	$-e^{i\pi\delta}$
------------	---	-------------------

Perform representation analysis for the first orbit.
For identity, it is trivial.



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$$\{2_y | 0 \frac{1}{2} 0\}$$

- $|1x\rangle$ is transformed into $-|2x\rangle$
- $|1y\rangle$ is transformed into $|2y\rangle$
- $|1z\rangle$ is transformed into $-|2z\rangle$

$$\begin{pmatrix} & & -1 & \\ & & & 1 \\ & & & & -1 \\ -1 & & & & \\ & 1 & & & \\ & & -1 & & \end{pmatrix}$$



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Decomposition into IRs

$$\eta(\Gamma_1) = \frac{1}{2}(6 \times 1 + 0 \times e^{i\pi\delta}) = 3$$

$$\eta(\Gamma_2) = \frac{1}{2}(6 \times 1 + 0 \times -e^{i\pi\delta}) = 3$$



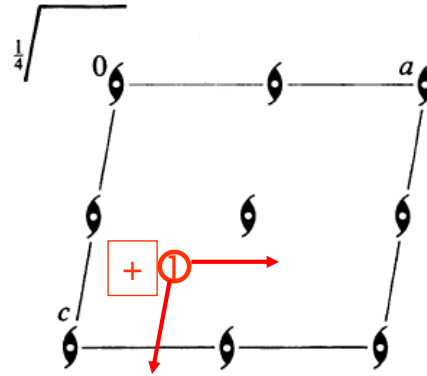
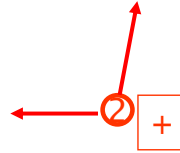
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Projection onto Γ_1

$$P|1x\rangle = |1x\rangle - e^{-i\pi\delta}|2x\rangle$$

$$P|1y\rangle = |1y\rangle + e^{-i\pi\delta}|2y\rangle$$

$$P|1z\rangle = |1z\rangle - e^{-i\pi\delta}|2z\rangle$$



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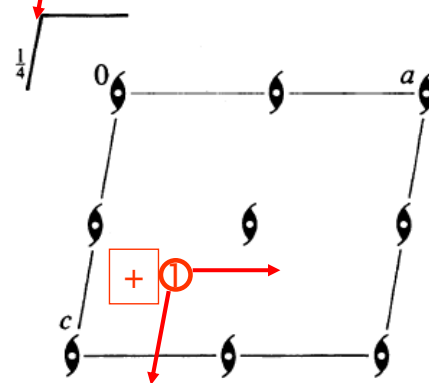
ISIS

Projection onto Γ_2

$$P|1x\rangle = |1x\rangle + e^{-i\pi\delta}|2x\rangle$$

$$P|1y\rangle = |1y\rangle - e^{-i\pi\delta}|2y\rangle$$

$$P|1z\rangle = |1z\rangle + e^{-i\pi\delta}|2z\rangle$$



The same can be done for the second orbit

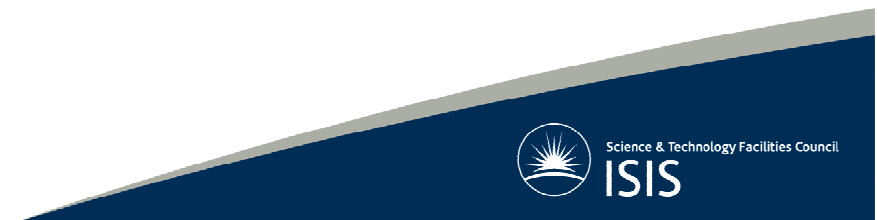


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Magnetic diffraction

L.C.Chapon
ISIS Facility, Rutherford Appleton
Laboratory, UK



Outline

- Nuclear scattering
- Magnetic scattering using a non-polarized neutron beam
- Type of magnetic structures (FStudio)
- Instrumentation



Scattering cross sections

Incident flux Φ of neutron of wavevector k .

Neutron is in the initial state λ

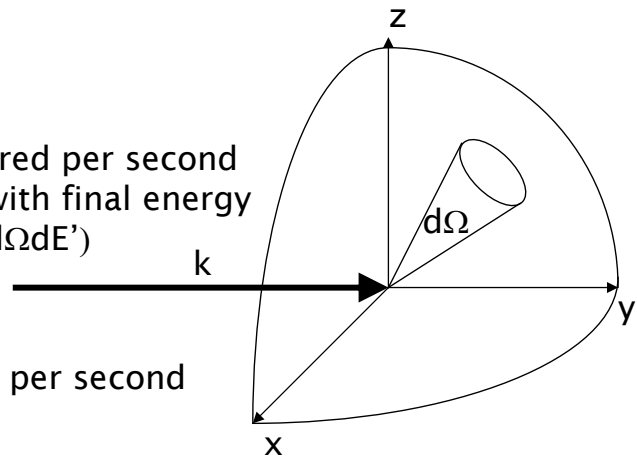
After scattering the neutron wavevector is k' and the neutron is in the state λ'

Partial differential cross section:

$$\frac{d^2\sigma}{d\Omega dE'} \quad \text{Number of neutrons scattered per second into a solid angle } d\Omega \text{ and with final energy between } E' \text{ and } E'+dE' / (\Phi d\Omega dE')$$

Differential cross section:

$$\frac{d\sigma}{d\Omega} \quad \text{Number of neutrons scattered per second into a solid angle } d\Omega / (\Phi d\Omega)$$



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Scattering cross sections

Incident neutron with wavevector k and state λ

Scattered neutron with wavevector k' and state λ'

In the Born approximation:

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{k'}{k} \left(\frac{m}{2\pi\hbar^2} \right)^2 \left| \langle k' \lambda' | V | k \lambda \rangle \right|^2 \delta(E_{\lambda'} - E_{\lambda} + E - E')$$



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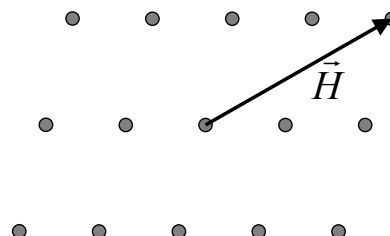
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Elastic nuclear scattering

In the Born approximation, the scattered intensity is given by:

The interaction between the neutron and the atomic nucleus is represented by the Fermi pseudo-potential, a scalar field.

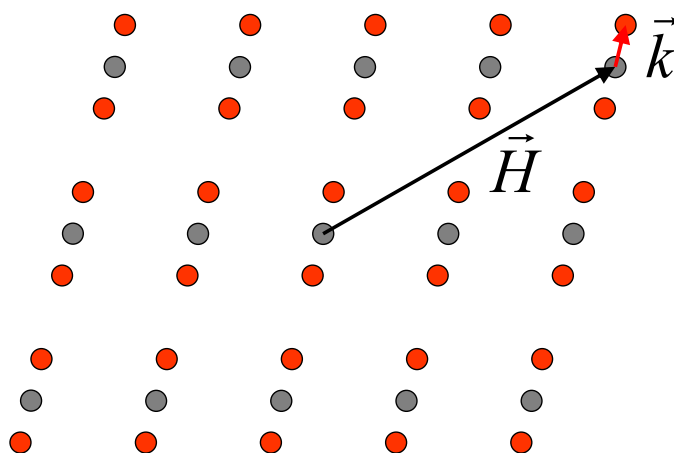
$$\frac{d\sigma}{d\Omega} =$$



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Elastic magnetic scattering



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Cross sections

In the magnetic case, we need to evaluate the matrix element :

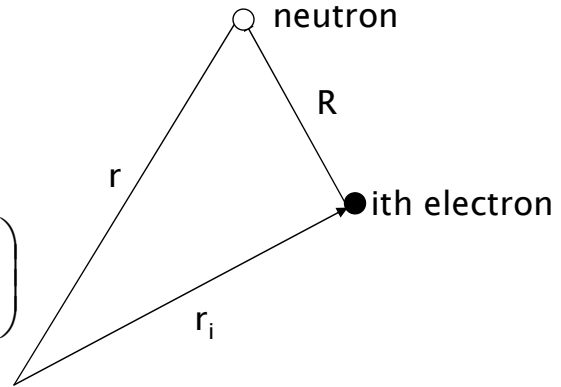
$$\langle k' \sigma' | V_m | k \sigma \rangle$$

$$A(R) = \frac{\mu_0}{4\pi} \frac{\mu_e \times \hat{R}}{R^2}$$

$$B = \text{curl} A = \nabla \times A$$

$$V = -\mu_n \cdot B = -\gamma \mu_N 2\mu_B \frac{\mu_0}{4\pi} \sigma \cdot \nabla \times \left(\frac{s \times \hat{R}}{R^2} \right)$$

$$\bar{\nabla} \times \left(\frac{\vec{s} \times \hat{R}}{R^2} \right) = \frac{1}{2\pi^2} \int \hat{q} \times \vec{s} \times \hat{q} e^{i\vec{q} \cdot \vec{R}} d\vec{q}$$



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The magnetic structure we will consider must have a moment distribution that can be expanded in Fourier series.

$$\vec{m}_{lj} = \sum_{\{k\}} \vec{S}_{kj} \cdot e^{-2\pi i \vec{k} \cdot \vec{R}_l}$$

Unit-cell magnetic structure factor:

$$\vec{M}(\vec{\kappa}) = p \sum_j f_j(\vec{\kappa}) \vec{S}_{kj} e^{2\pi i \vec{\kappa} \cdot \vec{r}_j}$$



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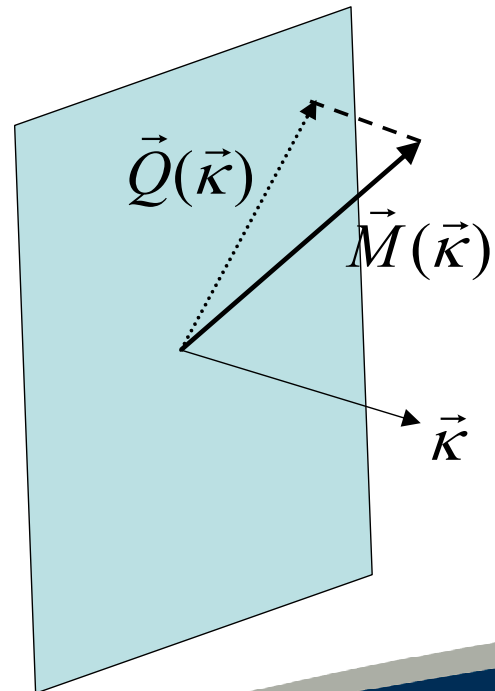
Magnetic interaction vector

Magnetic interaction vector:

$$\vec{Q}(\vec{k}) = \vec{k} \times \vec{M}(\vec{k}) \times \vec{k}$$

The intensity of a *magnetic Bragg peak* I :

$$I \propto \left| \vec{Q}(\vec{k}) \cdot \vec{Q}^*(\vec{k}) \right|$$

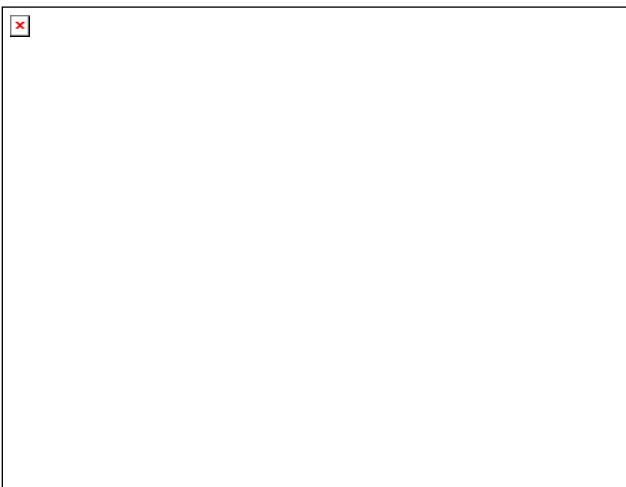


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Magnetic form factor

In the dipole approximation:

$$f(Q) = \langle j_0(Q) \rangle + \left(1 - \frac{2}{g}\right) \langle j_2(Q) \rangle$$



International Tables of Crystallography, Volume C,
ed. by AJC Wilson, Kluwer Ac. Pub., 1998, p. 513

<http://neutron.ornl.gov/~zhelud/useful/formfac/index.html>



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Notations

\vec{k} scattering vector

$\vec{M}(\vec{k})$ Magnetic structure factor

$\vec{Q}(\vec{k}) \equiv \vec{M}(\vec{k})_{\perp}$ Magnetic interaction vector

$\vec{\mu}_n$ magnetic dipole moment of the neutron

$$\mu_N = \frac{e\hbar}{2m_p} \text{ (nuclear magneton)}$$

$$\gamma = 1.913$$

μ_e magnetic dipole moment of the electron

$$\mu_B = \frac{e\hbar}{2m_e} \text{ (Bohr magneton)}$$



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Visualize magnetic structure with FStudio

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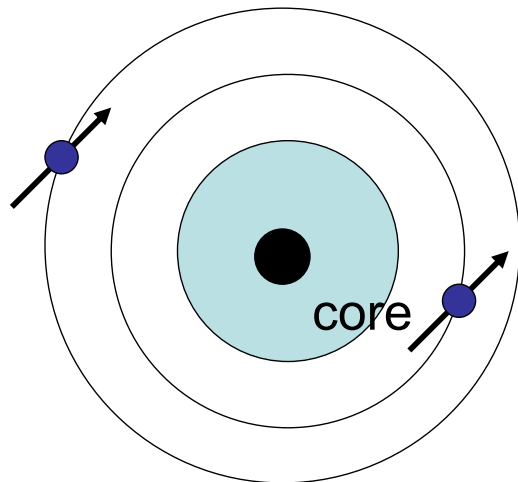


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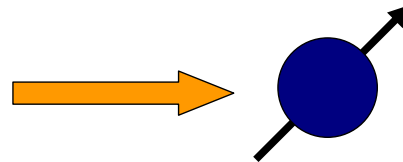
Ions with intrinsic magnetic moments

Atoms/ions with unpaired electrons



Ni²⁺

Intra-atomic electron correlation
Hund's rule: maximum S/J



$$\mathbf{m} = g_J \mathbf{J} \quad (\text{rare earths})$$

$$\mathbf{m} = g_S \mathbf{S} \quad (\text{transition metals})$$



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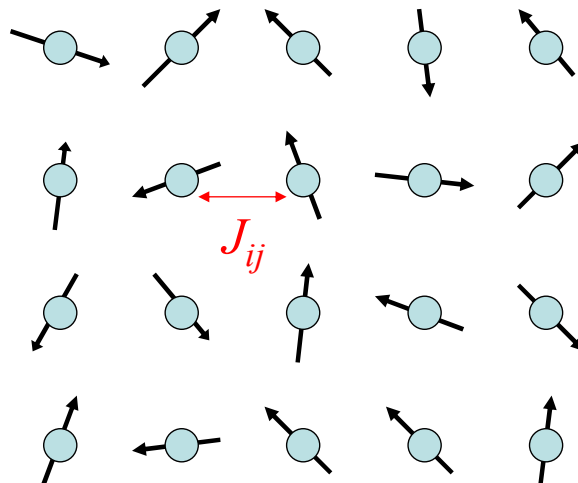
What is a magnetic structure?

Paramagnetic state:

Snapshot of magnetic moment configuration

$$E_{ij} = -J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$\langle \mathbf{S}_i \rangle = 0$$



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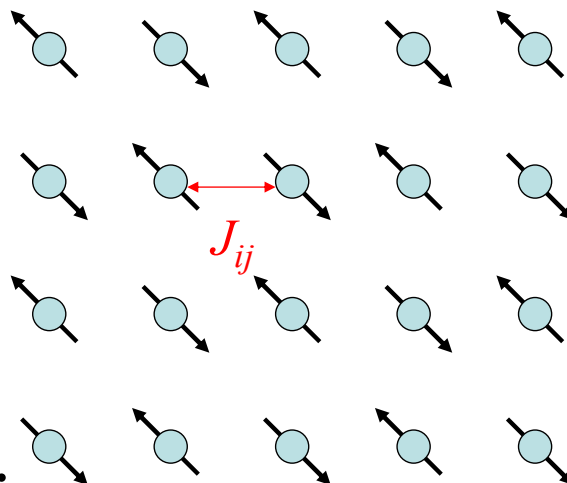
What is a magnetic structure?

Ordered state: Anti-ferromagnetic

Small fluctuations (spin waves) of the static configuration

$$E_{ij} = -J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$\langle \mathbf{S}_i \rangle \neq 0$$



Magnetic structure:

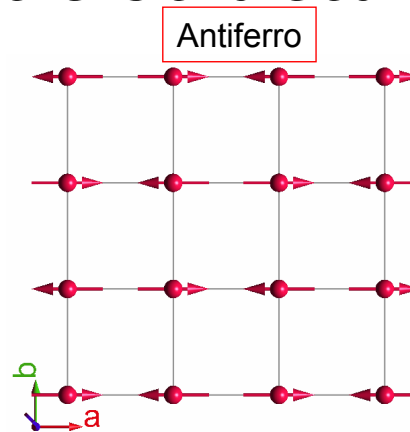
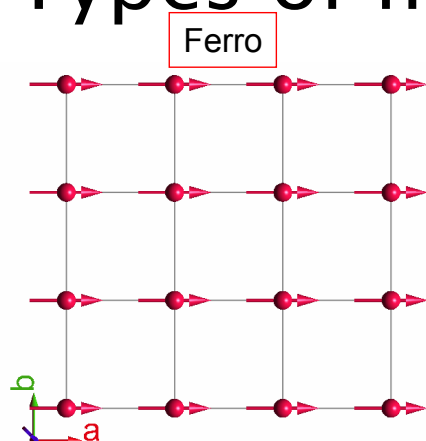
Quasi-static configuration of magnetic moments



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Types of magnetic structures



Very often magnetic structures are complex due to :

- competing exchange interactions (i.e. RKKY)
- geometrical frustration
- competition between exchange and single ion anisotropies

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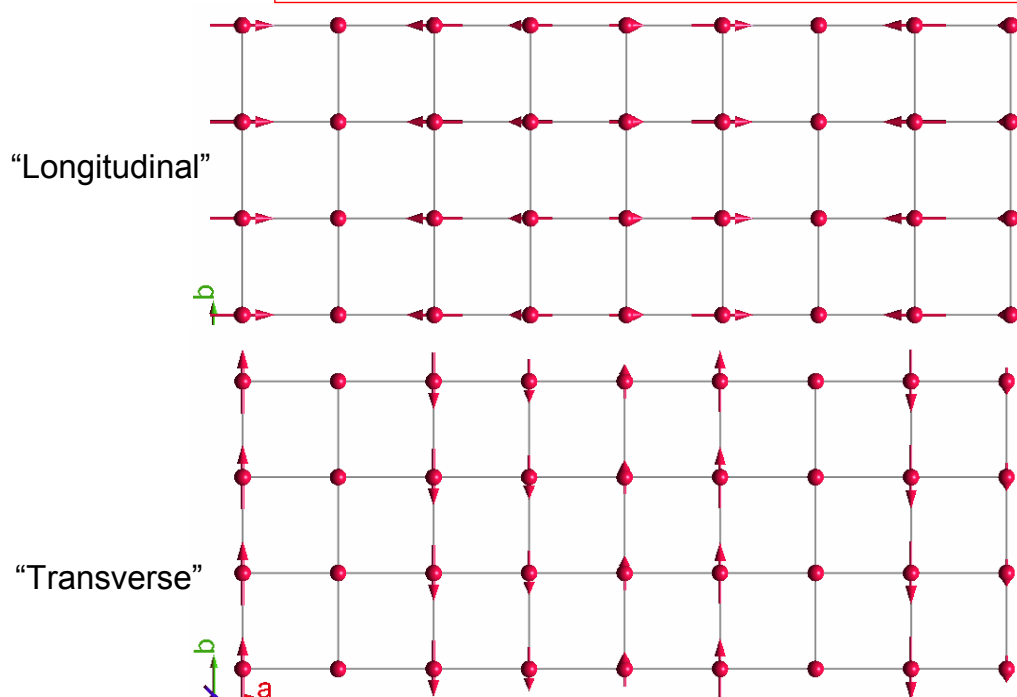


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Types of magnetic structures

Amplitude-modulated or Spin-Density Waves



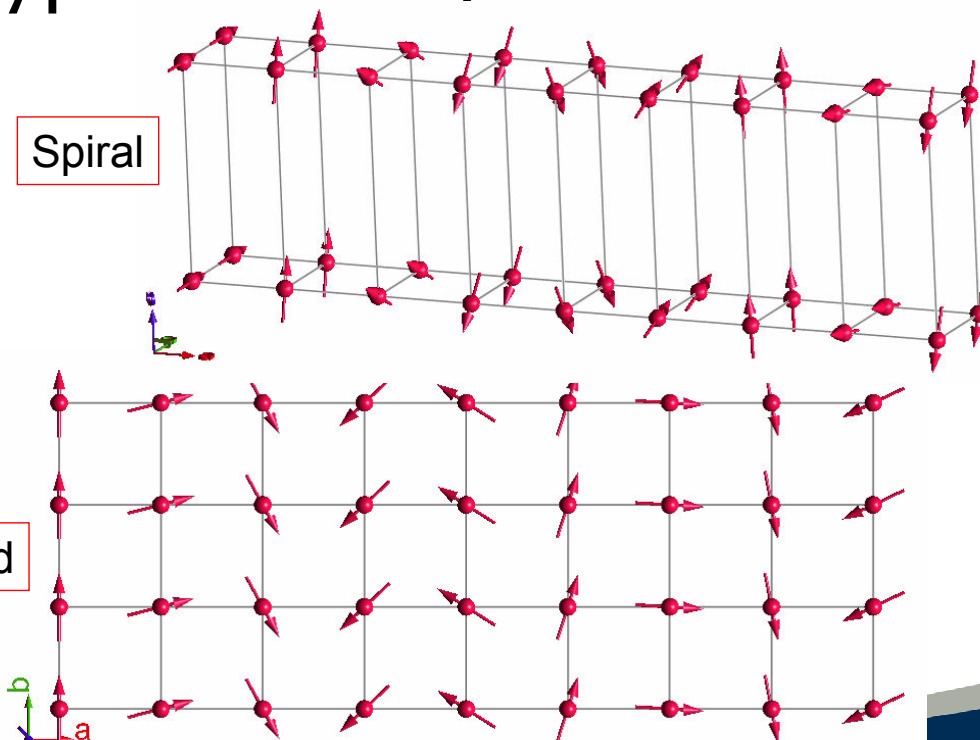
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Types of magnetic structures

Spiral

Cycloid

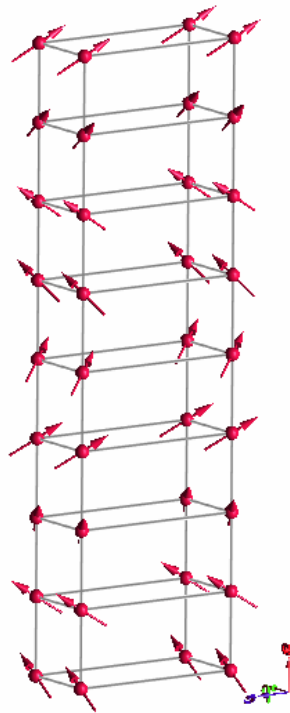


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Types of magnetic structures

Conical



Shubnikov magnetic groups, are limited to:

- Commensurate magnetic structure.
- Real representation of dimension 1.

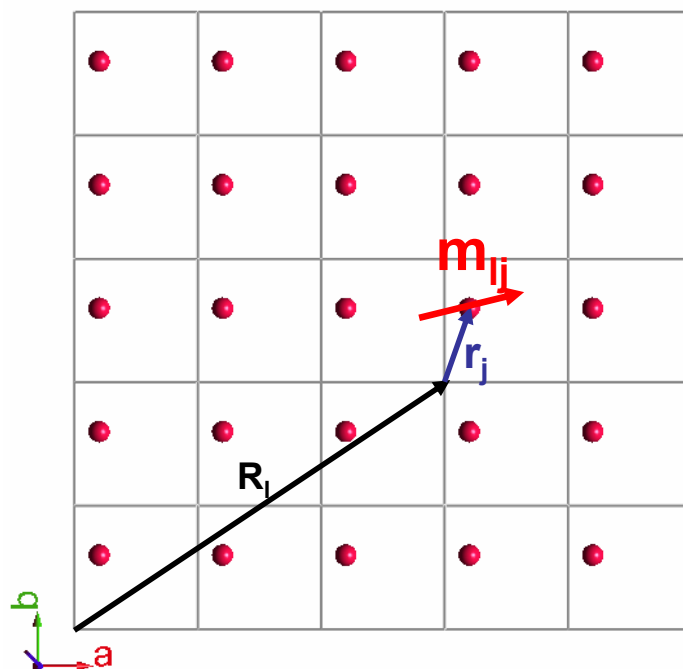


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Formalism of prop. Vector : Basics

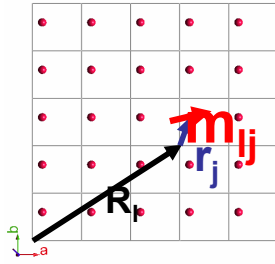
Position of atom j in unit-cell l is given by:

$R_{lj} = R_l + r_j$ where R_l is a pure lattice translation



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Formalism of prop. Vector : Basics



$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}j} \exp\{-2\pi i \mathbf{k} \mathbf{R}_l\}$$

$$\mathbf{R}_{lj} = \mathbf{R}_l + \mathbf{r}_j = l_1 \mathbf{a} + l_2 \mathbf{b} + l_3 \mathbf{c} + x_j \mathbf{a} + y_j \mathbf{b} + z_j \mathbf{c}$$

Necessary condition for real \mathbf{m}_{lj}

$$\mathbf{S}_{-\mathbf{k}j} = \mathbf{S}_{\mathbf{k}j}^*$$

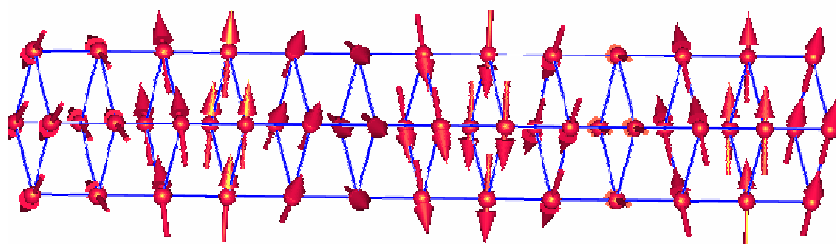


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Formalism of prop. Vector : Basics

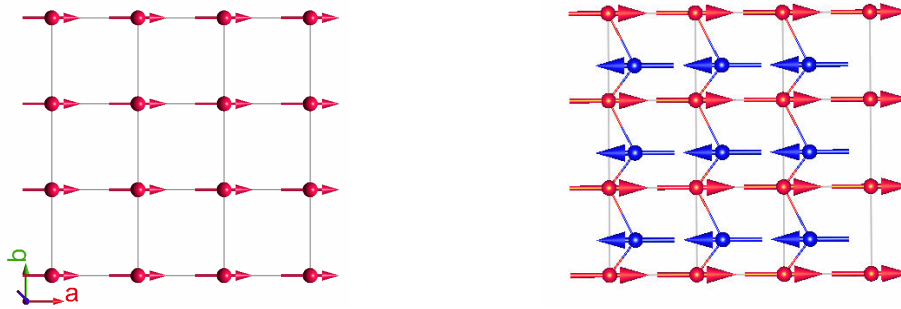
A magnetic structure is fully described by:

- Wave-vector(s) $\{\mathbf{k}\}$.
- Fourier components $\mathbf{S}_{\mathbf{k}j}$ for each magnetic atom j and wave-vector \mathbf{k} .
 $\mathbf{S}_{\mathbf{k}j}$ is a complex vector (6 components) !!!
- Phase for each magnetic atom j , Φ_{kj}



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Single propagation vector $\mathbf{k} = (0,0,0)$



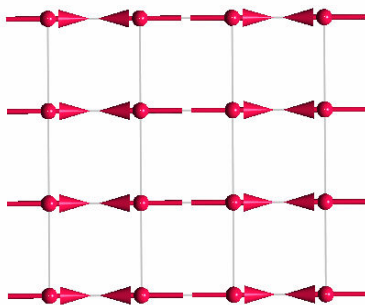
$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}j} \exp\{-2\pi i \mathbf{k} \mathbf{R}_l\} = \mathbf{S}_{\mathbf{k}j}$$

- The magnetic structure may be described within the crystallographic unit cell
- Magnetic symmetry: conventional crystallography plus time reversal operator: crystallographic magnetic groups



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Single propagation vector $\mathbf{k} = 1/2 \text{ H}$



$$\mathbf{m}_{lj} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}j} \exp\{-2\pi i \mathbf{k} \mathbf{R}_l\} = \mathbf{S}_{\mathbf{k}j} (-1)^{n(l)}$$

REAL Fourier coefficients \equiv magnetic moments

The magnetic symmetry may also be described using crystallographic magnetic space groups



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Fourier coef. of sinusoidal structures

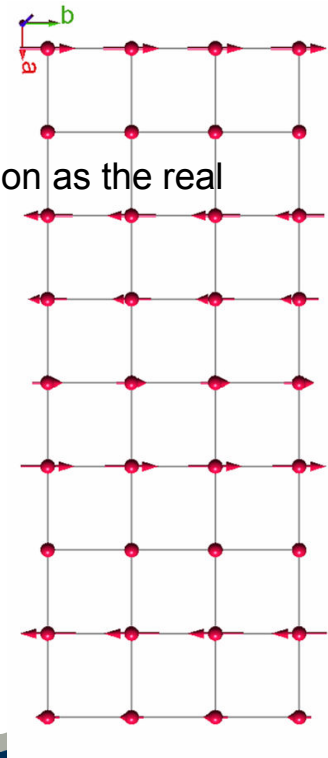
- \mathbf{k} interior of the Brillouin zone (pair \mathbf{k} , $-\mathbf{k}$)

- Real $\mathbf{S}_{\mathbf{k}}$, or imaginary component in the same direction as the real one

$$\mathbf{m}_{lj} = \mathbf{S}_{\mathbf{k}j} \exp(-2\pi i \mathbf{k} \mathbf{R}_l) + \mathbf{S}_{-\mathbf{k}j} \exp(2\pi i \mathbf{k} \mathbf{R}_l)$$

$$\mathbf{S}_{\mathbf{k}j} = \frac{1}{2} m_j \mathbf{u}_j \exp(-2\pi i \phi_{\mathbf{k}j})$$

$$\mathbf{m}_{lj} = m_j \mathbf{u}_j \cos 2\pi(\mathbf{k} \mathbf{R}_l + \phi_{\mathbf{k}j})$$



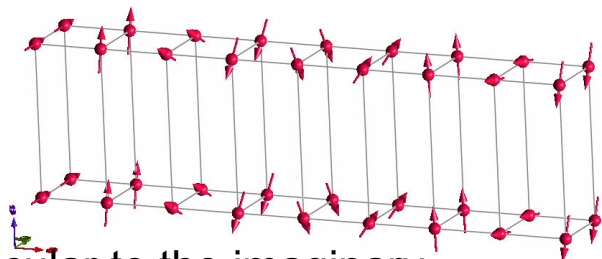
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Fourier coefficients of helical structures

- \mathbf{k} interior of the Brillouin zone

- Real component of $\mathbf{S}_{\mathbf{k}}$ perpendicular to the imaginary component



$$\mathbf{S}_{\mathbf{k}j} = \frac{1}{2} \left[m_{uj} \mathbf{u}_j + i m_{vj} \mathbf{v}_j \right] \exp(-2\pi i \phi_{\mathbf{k}j})$$

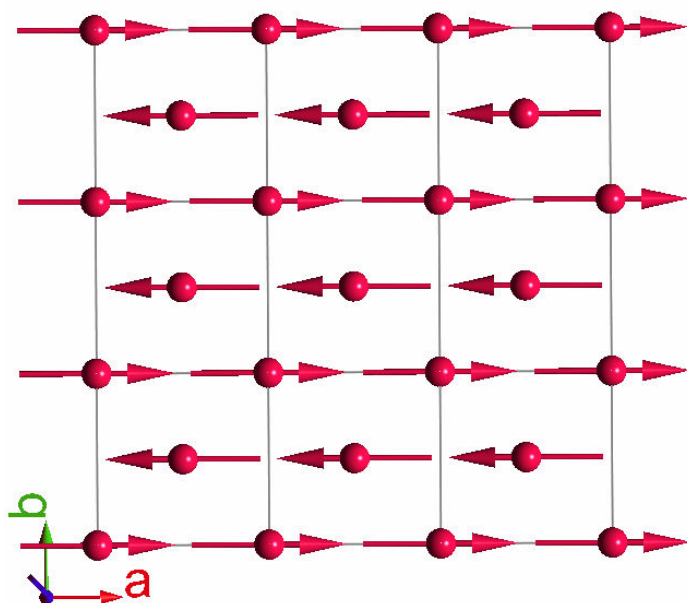
$$\mathbf{m}_{lj} = m_{uj} \mathbf{u}_j \cos 2\pi(\mathbf{k} \mathbf{R}_l + \phi_{\mathbf{k}j}) + m_{vj} \mathbf{v}_j \sin 2\pi(\mathbf{k} \mathbf{R}_l + \phi_{\mathbf{k}j})$$



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Centred cells!



$k=(1,0,0)$ or $(0,1,0)$!!!!!



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Examples. Fstudio



www.ill.fr/dif

Type of lattice P, C, I, F.....

{
LATTICE P

Propagation vector(s)

K 0.5 0.0 0.0

SYMM x,y,z

MSYM u,v,w,0.0

List of symmetry operators with associated magnetic operator

MATOM Ce1 CE 0.0 0.0 0.0

Magnetic atom

SKP 1 1 2.0 0.0 0.0 0.0 0.0 0.0 0.0

Fourier coefficients and phase

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